



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 03:21 AM UTC

PDB ID : 9LJ2 / pdb_00009lj2
EMDB ID : EMD-63131
Title : Structure of isw1-nucleosome double-bound complex in ADP-ADP+ state
Authors : Sia, Y.; Pan, H.; Chen, Z.
Deposited on : 2025-01-14
Resolution : 2.98 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

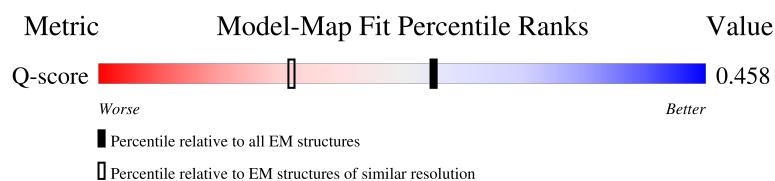
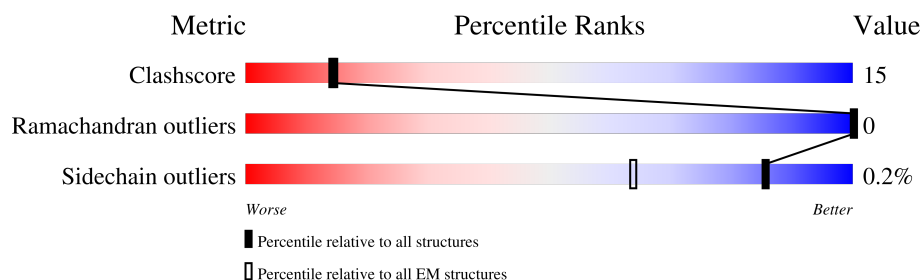
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



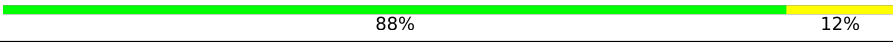
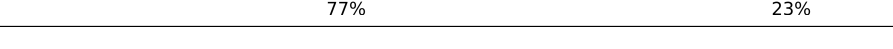
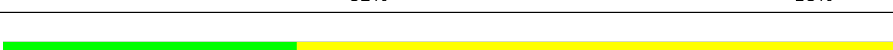
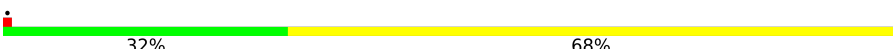
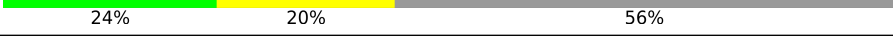
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13236 (2.48 - 3.48)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	98	 80% 20%
1	E	98	 72% 24%
2	B	88	 6% 75% 24%
2	F	88	 7% 69% 31%

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Mol	Chain	Length	Quality of chain
3	C	107	 80%20%
3	G	107	 88%12%
4	D	93	 77%23%
4	H	93	 82%18%
5	I	147	 33%67%
6	J	147	 32%68%
7	K	1129	 13%33%20%47%
7	N	1129	 13%24%20%56%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21131 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			801	506	153	139	3		
1	E	95	Total	C	N	O	S	0	0
			779	492	148	136	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	87	Total	C	N	O	S	0	0
			703	443	142	117	1		
2	F	88	Total	C	N	O	S	0	0
			708	445	143	119	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total	C	N	O	0	0
			811	510	158	143		
3	G	107	Total	C	N	O	0	0
			815	513	159	143		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
4	H	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

- Molecule 5 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	147	Total	C	N	O	P	0	0
			3002	1428	543	884	147		

- Molecule 6 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	147	Total	C	N	O	P	0	0
			3025	1435	563	880	147		

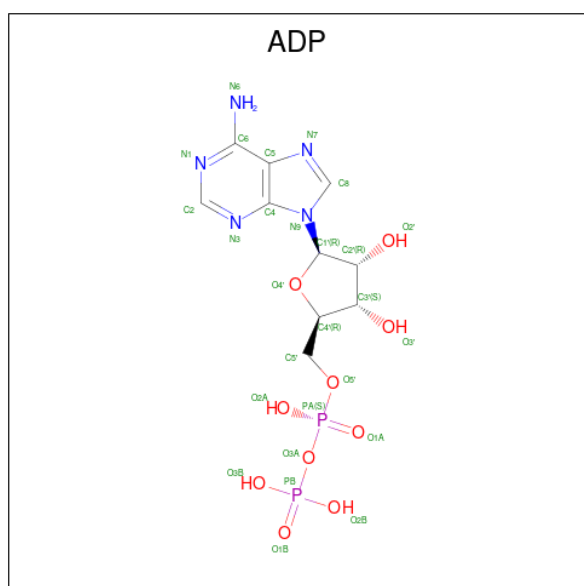
- Molecule 7 is a protein called ISWI chromatin-remodeling complex ATPase ISW1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	598	Total	C	N	O	S	0	0
			4921	3144	845	919	13		
7	N	495	Total	C	N	O	S	0	0
			4066	2604	699	750	13		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	K	1	Total	Mg	0
			1	1	
8	N	1	Total	Mg	0
			1	1	

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

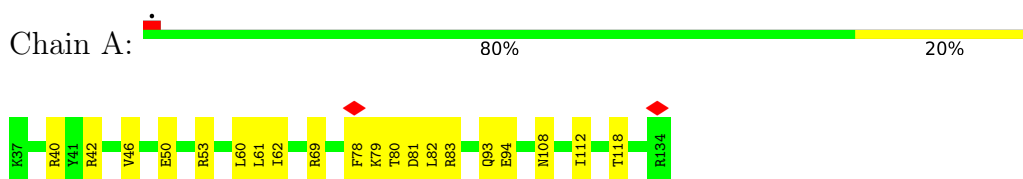


Mol	Chain	Residues	Atoms					AltConf
9	K	1	Total 27	C 10	N 5	O 10	P 2	0
9	N	1	Total 27	C 10	N 5	O 10	P 2	0

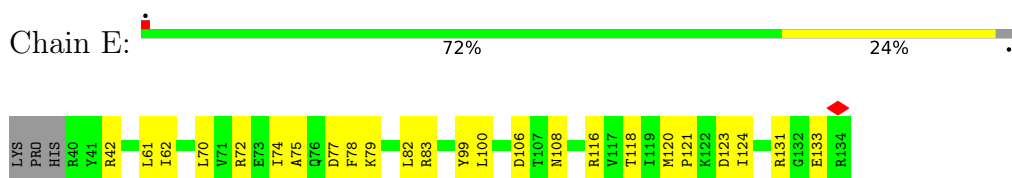
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

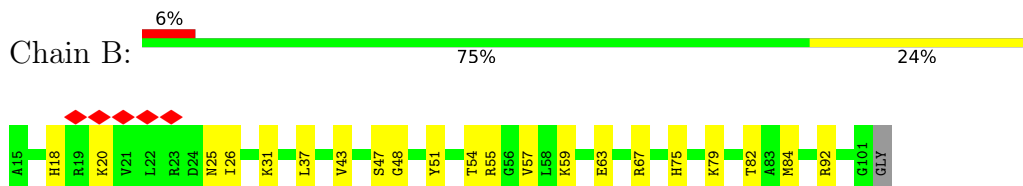
- Molecule 1: Histone H3



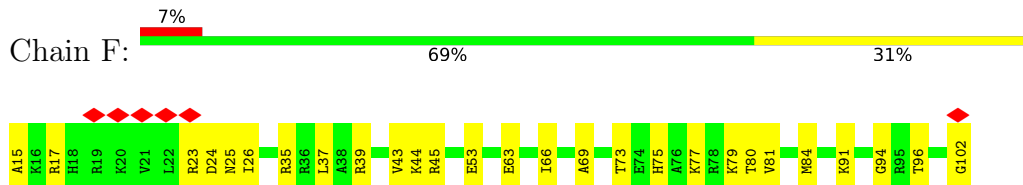
- Molecule 1: Histone H3



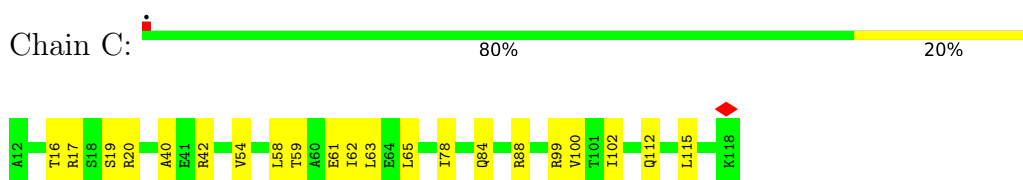
- Molecule 2: Histone H4



- Molecule 2: Histone H4

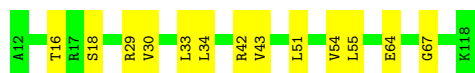


- Molecule 3: Histone H2A



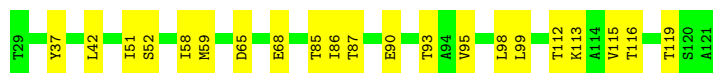
- Molecule 3: Histone H2A

Chain G:  88% 12%



- Molecule 4: Histone H2B

Chain D:  77% 23%

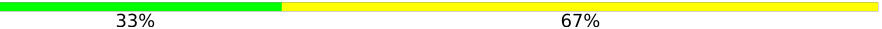


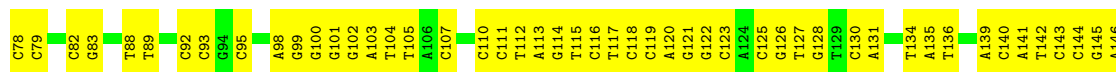
- Molecule 4: Histone H2B

Chain H:  82% 18%



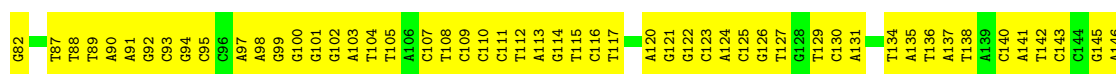
- Molecule 5: DNA (147-MER)

Chain I:  33% 67%



- Molecule 6: DNA (147-MER)

Chain J:  32% 68%



- Molecule 7: ISWI chromatin-remodeling complex ATPase ISW1

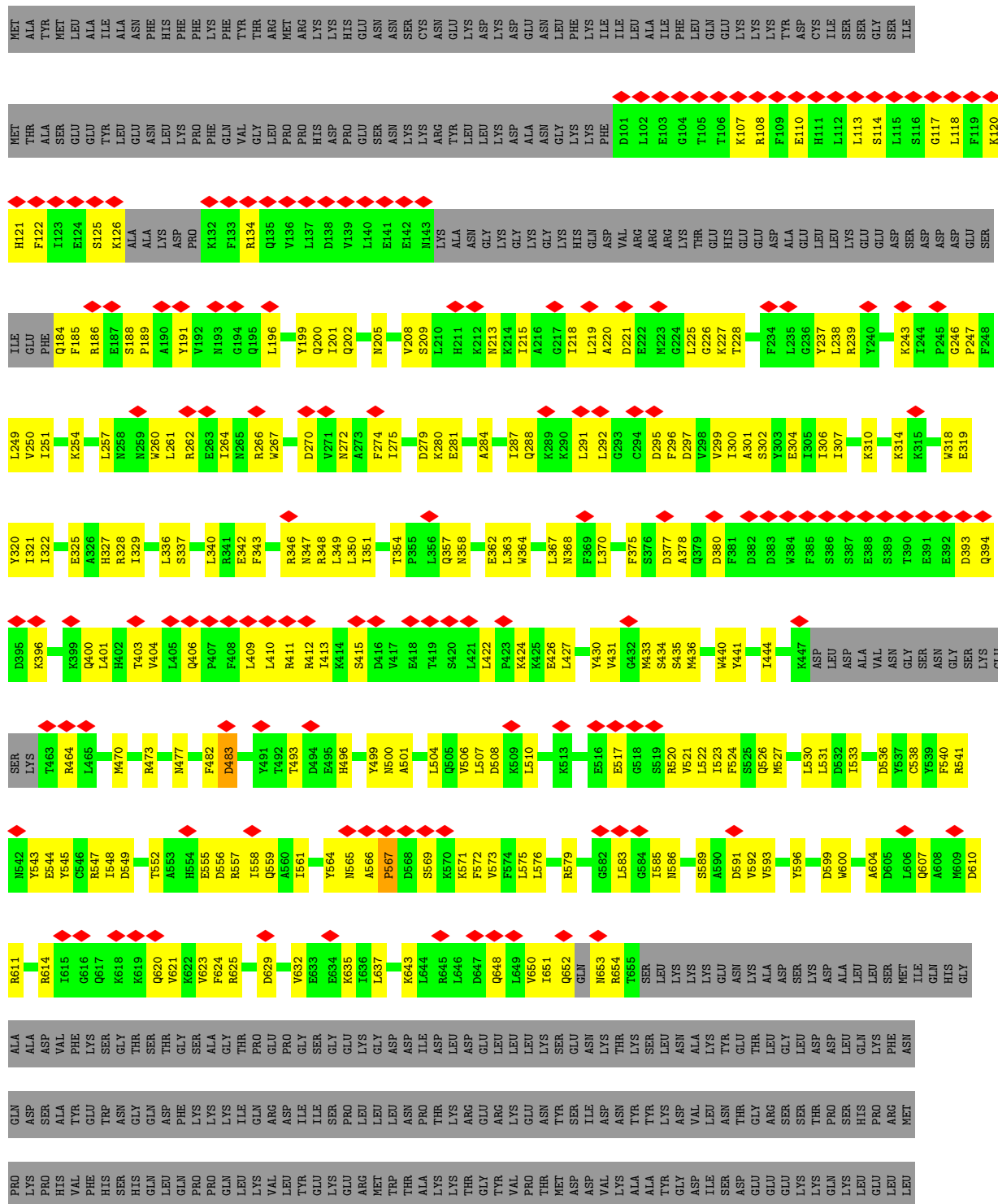
Chain K:  13% 33% 20% 47%

PHE	ASP	ILE	ALA	LEU	ASP	LEU	LEU	ASP	PRO	H634	R557	M469	D395	Q195	R134	MET
ASP	ARG	GLU	ASP	TYR	ILE	LEU	LEU	ILE	GLY	K635	R558	M469	K396	L196	Q135	THR
PHE	ILE	TYR	TRP	GLY	ILE	SER	GLY	ILE	SER	I636	I558	R473	I397	P197	V136	ALA
ILE	LEU	GLY	GLY	GLY	PRO	GLY	GLY	PRO	GLY	I637	Y564	R473	V398	GLU	L137	SER
VAL	LEU	LYS	GLY	ARG	LEU	ARG	MET	LEU	LYS	E638	Y565	N477	K399	GLU	D138	ALA
LEU	MET	TYR	GLY	MET	LEU	TRP	TRP	LEU	GLY	R639	A566	H478	Q400	TYR	V139	ILE
ASP	PHE	LEU	THR	THR	L764	P765	P766	P767	D704	K643	P567	P479	H402	LEU	L140	ALA
ASP	THR	THR	THR	THR	N765	N766	N767	N768	D705	L644	D568	D483	Q406	LEU	E141	ASN
ALA	ALA	ALA	ALA	LYS	P766	P766	P766	P766	D706	R645	S569	D483	Q406	LEU	E142	THR
LYS	GLY	LYS	LYS	LYS	L646	L646	L646	L646	D707	D647	K570	T493	P407	LEU	L71	THR
THR	THR	THR	THR	THR	G648	G648	G648	G648	D708	L708	K571	T493	P407	LEU	K72	ARG
GLY	GLY	GLY	GLY	GLY	L649	L649	L649	L649	D709	L649	E495	D494	L409	LEU	P73	LYS
VAL	VAL	VAL	VAL	VAL	V650	V650	V650	V650	E710	V651	F574	E495	L409	LEU	F74	PHE
PRO	PRO	PRO	PRO	PRO	L576	L576	L576	L576	E711	L576	L576	E495	L409	LEU	F74	THR
LYS	LYS	LYS	LYS	LYS	L576	L576	L576	L576	L711	L576	L576	E495	L409	LEU	Q75	ARG
THR	THR	THR	THR	THR	L712	L712	L712	L712	L712	L712	L712	E495	L409	LEU	V76	MET
MET	MET	MET	MET	MET	L713	L713	L713	L713	L713	L713	L713	E495	L409	LEU	V76	ARG
ASP	ASP	ASP	ASP	ASP	L714	L714	L714	L714	L714	L714	L714	E495	L409	LEU	L78	LYS
GLY	GLY	GLY	GLY	GLY	S715	S715	S715	S715	S715	S715	S715	E495	L409	LEU	P79	GLY
ILE	ILE	ILE	ILE	ILE	E716	E716	E716	E716	E716	E716	E716	E495	L409	LEU	P80	ASN
GLY	GLY	GLY	GLY	GLY	N717	N717	N717	N717	N717	N717	N717	E495	L409	LEU	H81	ASN
ASP	ASP	ASP	ASP	ASP	K718	K718	K718	K718	K718	K718	K718	E495	L409	LEU	D82	ASN
ASN	ASN	ASN	ASN	ASN	T719	T719	T719	T719	T719	T719	T719	E495	L409	LEU	P83	SER
TYR	TYR	TYR	TYR	TYR	K720	K720	K720	K720	K720	K720	K720	E495	L409	LEU	E84	CYS
LYS	LYS	LYS	LYS	LYS	S721	S721	S721	S721	S721	S721	S721	E495	L409	LEU	N86	ASN
ASP	ASP	ASP	ASP	ASP	L722	L722	L722	L722	L722	L722	L722	E495	L409	LEU	K87	GLY
VAL	VAL	VAL	VAL	VAL	N723	N723	N723	N723	N723	N723	N723	E495	L409	LEU	K88	LYS
LEU	LEU	LEU	LEU	LEU	L724	L724	L724	L724	L724	L724	L724	E495	L409	LEU	R89	ASP
THR	THR	THR	THR	THR	K725	K725	K725	K725	K725	K725	K725	E495	L409	LEU	L92	LYS
GLY	GLY	GLY	GLY	GLY	Y726	Y726	Y726	Y726	Y726	Y726	Y726	E495	L409	LEU	K93	ASP
ARG	ARG	ARG	ARG	ARG	E727	E727	E727	E727	E727	E727	E727	E495	L409	LEU	D94	ASN
ASN	ASN	ASN	ASN	ASN	L728	L728	L728	L728	L728	L728	L728	E495	L409	LEU	A95	PHE
LYS	LYS	LYS	LYS	LYS	T729	T729	T729	T729	T729	T729	T729	E495	L409	LEU	N96	ILE
GLY	GLY	GLY	GLY	GLY	G730	G730	G730	G730	G730	G730	G730	E495	L409	LEU	G97	ILE
LEU	LEU	LEU	LEU	LEU	L731	L731	L731	L731	L731	L731	L731	E495	L409	LEU	K98	LEU
PRO	PRO	PRO	PRO	PRO	D732	D732	D732	D732	D732	D732	D732	E495	L409	LEU	X99	ALA
ALA	ALA	ALA	ALA	ALA	L733	L733	L733	L733	L733	L733	L733	E495	L409	LEU	F100	ILE
ASP	ASP	ASP	ASP	ASP	L734	L734	L734	L734	L734	L734	L734	E495	L409	LEU	D101	PHE
VAL	VAL	VAL	VAL	VAL	Q735	Q735	Q735	Q735	Q735	Q735	Q735	E495	L409	LEU	L102	GLN
LYS	LYS	LYS	LYS	LYS	P736	P736	P736	P736	P736	P736	P736	E495	L409	LEU	E103	GLY
GLY	GLY	GLY	GLY	GLY	K737	K737	K737	K737	K737	K737	K737	E495	L409	LEU	G104	LYS
THR	THR	THR	THR	THR	L738	L738	L738	L738	L738	L738	L738	E495	L409	LEU	I108	LYS
ASN	ASN	ASN	ASN	ASN	N739	N739	N739	N739	N739	N739	N739	E495	L409	LEU	R108	TYR
PRO	PRO	PRO	PRO	PRO	Q739	Q739	Q739	Q739	Q739	Q739	Q739	E495	L409	LEU	L118	ASP
VAL	VAL	VAL	VAL	VAL	D740	D740	D740	D740	D740	D740	D740	E495	L409	LEU	Q184	CYS
GLY	GLY	GLY	GLY	GLY	S741	S741	S741	S741	S741	S741	S741	E495	L409	LEU	F185	ILE
ASN	ASN	ASN	ASN	ASN	L742	L742	L742	L742	L742	L742	L742	E495	L409	LEU	H121	SER
THR	THR	THR	THR	THR	Y743	Y743	Y743	Y743	Y743	Y743	Y743	E495	L409	LEU	F122	GLY
LYS	LYS	LYS	LYS	LYS	E744	E744	E744	E744	E744	E744	E744	E495	L409	LEU	I123	SER
PRO	PRO	PRO	PRO	PRO	L745	L745	L745	L745	L745	L745	L745	E495	L409	LEU	E124	GLY
GLN	GLN	GLN	GLN	GLN	N746	N746	N746	N746	N746	N746	N746	E495	L409	LEU	A127	SER
LEU	LEU	LEU	LEU	LEU	G747	G747	G747	G747	G747	G747	G747	E495	L409	LEU	A128	GLY
LYS	LYS	LYS	LYS	LYS	Q748	Q748	Q748	Q748	Q748	Q748	Q748	E495	L409	LEU	K129	SER
VAL	VAL	VAL	VAL	VAL	D749	D749	D749	D749	D749	D749	D749	E495	L409	LEU	P131	GLY
GLY	GLY	GLY	GLY	GLY	F750	F750	F750	F750	F750	F750	F750	E495	L409	LEU	K132	SER
THR	THR	THR	THR	THR	K751	K751	K751	K751	K751	K751	K751	E495	L409	LEU	F133	ILE
GLU	GLU	GLU	GLU	GLU	L752	L752	L752	L752	L752	L752	L752	E495	L409	LEU		
GLN	GLN	GLN	GLN	GLN	LYS	LYS	LYS	LYS	LYS	LYS	LYS	E495	L409	LEU		
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	E495	L409	LEU		

LEU
VAL
ALA
GLU
LYS
ILE
PRO
GLU
ASN
THR
THR
HIS

● Molecule 7: ISWI chromatin-remodeling complex ATPase ISW1

Chain N: 



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154464	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.352	Depositor
Minimum map value	-0.141	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.075	Depositor
Map size ($\text{\AA}$)	346.4, 346.4, 346.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/813	0.49	0/1093
1	E	0.26	0/789	0.46	0/1059
2	B	0.25	0/711	0.45	0/950
2	F	0.26	0/716	0.44	0/955
3	C	0.23	0/821	0.39	0/1112
3	G	0.23	0/825	0.42	0/1116
4	D	0.23	0/729	0.46	0/985
4	H	0.23	0/737	0.41	0/993
5	I	0.25	0/3364	0.43	0/5187
6	J	0.26	0/3396	0.41	0/5242
7	K	0.20	0/5015	0.45	1/6758 (0.0%)
7	N	0.19	0/4142	0.43	1/5587 (0.0%)
All	All	0.23	0/22058	0.43	2/31037 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	567	PRO	CA-N-CD	-9.32	98.95	112.00
7	K	418	GLU	N-CA-C	-5.36	108.50	114.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	801	0	831	24	0
1	E	779	0	815	22	0
2	B	703	0	757	19	0
2	F	708	0	760	27	0
3	C	811	0	849	20	0
3	G	815	0	860	12	0
4	D	718	0	725	19	0
4	H	726	0	747	16	0
5	I	3002	0	1654	108	0
6	J	3025	0	1652	108	0
7	K	4921	0	4962	159	0
7	N	4066	0	4121	168	0
8	K	1	0	0	0	0
8	N	1	0	0	0	0
9	K	27	0	12	2	0
9	N	27	0	12	2	0
All	All	21131	0	18757	611	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 611 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LYS:NZ	2:B:63:GLU:OE2	2.08	0.86
7:N:322:ILE:HG22	7:N:349:LEU:HB3	1.58	0.84
7:K:330:LYS:HB2	7:K:362:GLU:HG3	1.59	0.83
5:I:92:DC:O2	6:J:56:DG:N2	2.12	0.83
7:N:196:LEU:HD23	7:N:201:ILE:HG13	1.61	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
1	E	93/98 (95%)	92 (99%)	1 (1%)	0	100	100
2	B	85/88 (97%)	78 (92%)	7 (8%)	0	100	100
2	F	86/88 (98%)	79 (92%)	7 (8%)	0	100	100
3	C	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
3	G	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
4	D	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
4	H	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
7	K	588/1129 (52%)	524 (89%)	64 (11%)	0	100	100
7	N	485/1129 (43%)	438 (90%)	47 (10%)	0	100	100
All	All	1825/3030 (60%)	1679 (92%)	146 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/86 (98%)	84 (100%)	0	100	100
1	E	82/86 (95%)	82 (100%)	0	100	100
2	B	72/72 (100%)	72 (100%)	0	100	100
2	F	72/72 (100%)	72 (100%)	0	100	100
3	C	81/84 (96%)	81 (100%)	0	100	100
3	G	82/84 (98%)	82 (100%)	0	100	100
4	D	77/79 (98%)	77 (100%)	0	100	100
4	H	79/79 (100%)	79 (100%)	0	100	100
7	K	546/1020 (54%)	544 (100%)	2 (0%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	N	452/1020 (44%)	451 (100%)	1 (0%)	87	92
All	All	1627/2682 (61%)	1624 (100%)	3 (0%)	85	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	K	420	SER
7	K	421	LEU
7	N	483	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
7	K	379	GLN
7	N	121	HIS
7	N	554	HIS
7	N	347	ASN
7	K	607	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ADP	K	1202	8	28,29,29	1.39	4 (14%)	43,45,45	1.86	9 (20%)
9	ADP	N	1202	8	28,29,29	1.43	4 (14%)	43,45,45	1.80	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	K	1202	8	-	5/16/32/32	0/3/3/3
9	ADP	N	1202	8	-	1/16/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	1202	ADP	C5-C4	4.77	1.47	1.39
9	K	1202	ADP	C5-C4	4.58	1.47	1.39
9	N	1202	ADP	C5-C6	2.68	1.48	1.41
9	K	1202	ADP	C5-C6	2.64	1.48	1.41
9	N	1202	ADP	C5-N7	-2.35	1.34	1.39

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	1202	ADP	C5-C4-N3	-5.91	118.58	126.72
9	N	1202	ADP	C5-C4-N3	-5.82	118.70	126.72
9	K	1202	ADP	N3-C4-N9	4.71	135.18	127.17
9	N	1202	ADP	N3-C4-N9	4.50	134.83	127.17
9	K	1202	ADP	C2-N3-C4	3.65	120.75	111.83

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	K	1202	ADP	C4'-C5'-O5'-PA
9	K	1202	ADP	C2'-C1'-N9-C4

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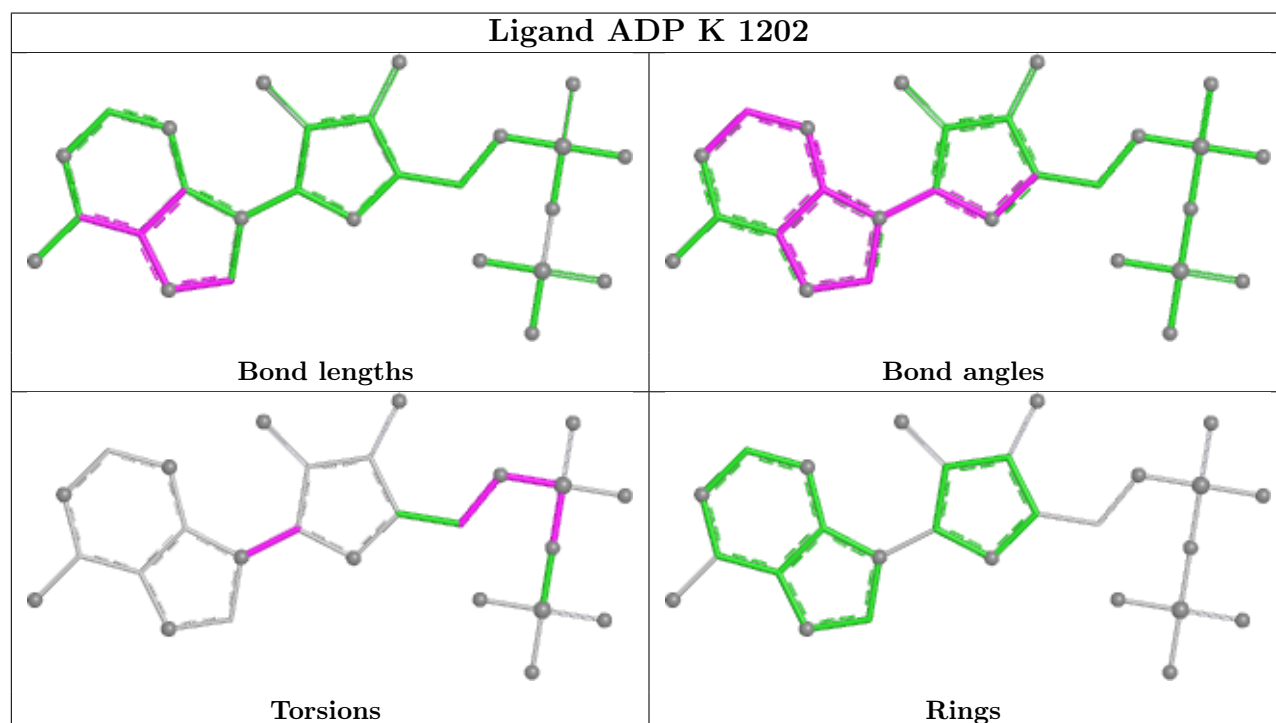
Mol	Chain	Res	Type	Atoms
9	K	1202	ADP	C2'-C1'-N9-C8
9	N	1202	ADP	O4'-C4'-C5'-O5'
9	K	1202	ADP	C5'-O5'-PA-O2A

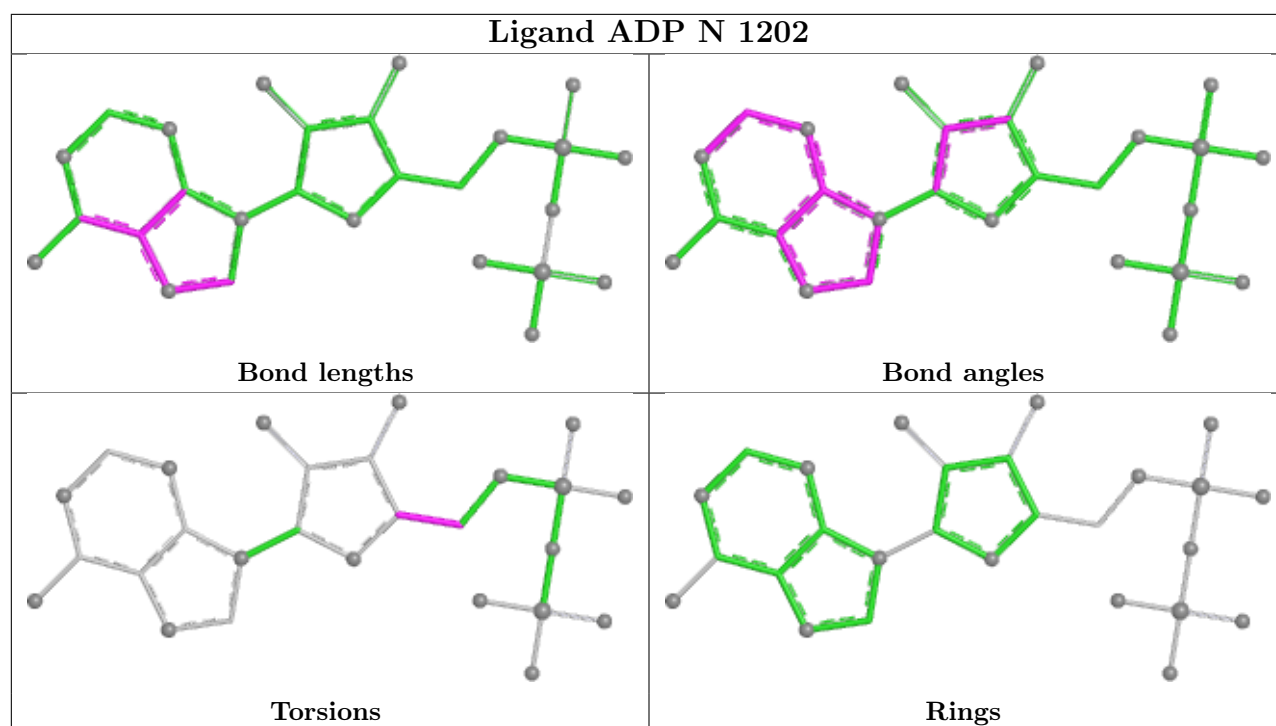
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	K	1202	ADP	2	0
9	N	1202	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

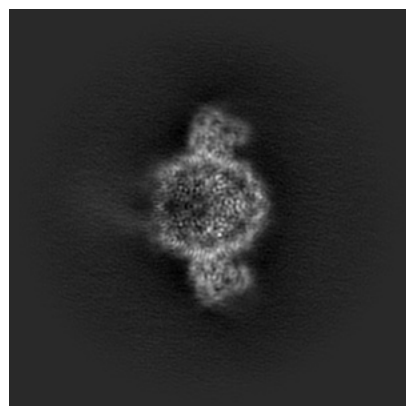
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63131. These allow visual inspection of the internal detail of the map and identification of artifacts.

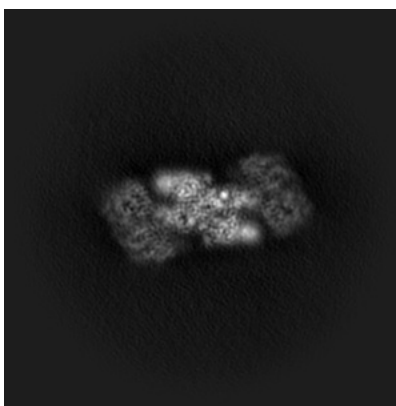
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

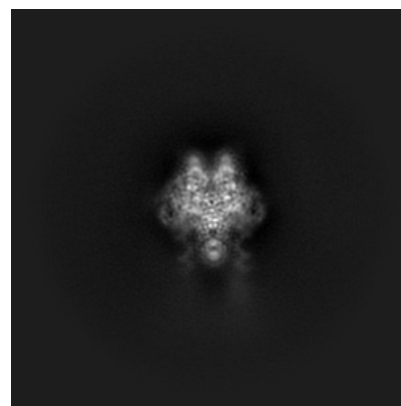
6.1.1 Primary map



X

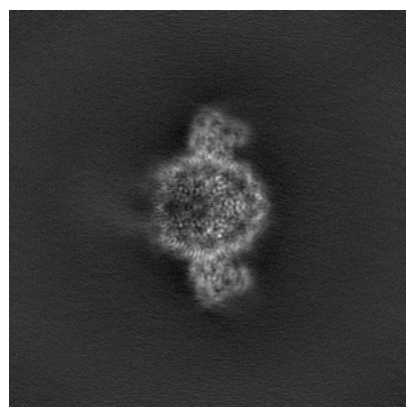


Y

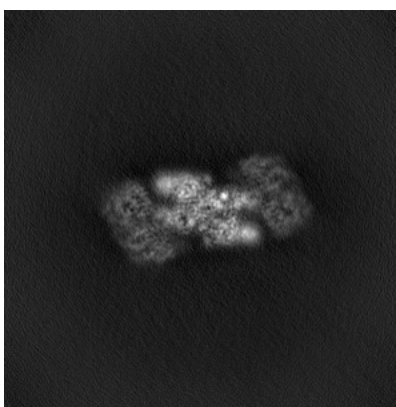


Z

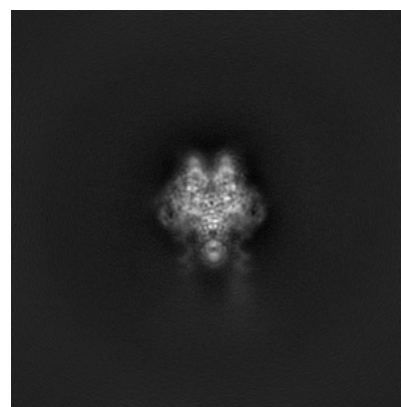
6.1.2 Raw map



X



Y

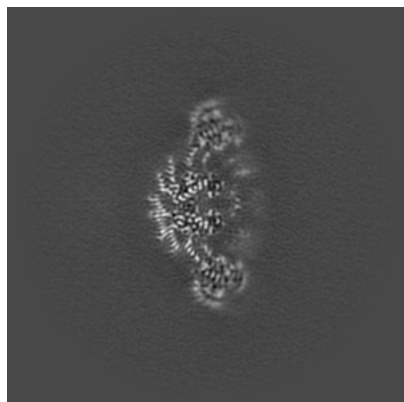


Z

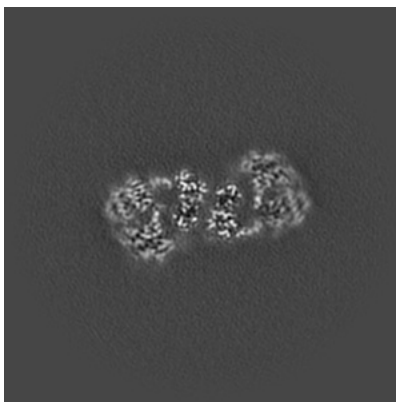
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

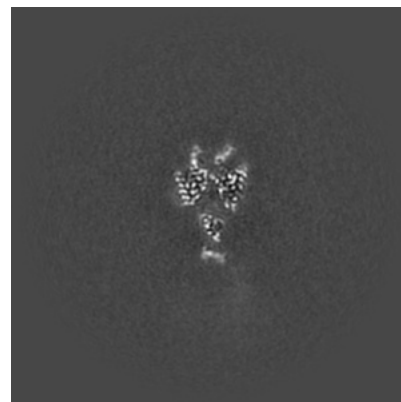
6.2.1 Primary map



X Index: 160

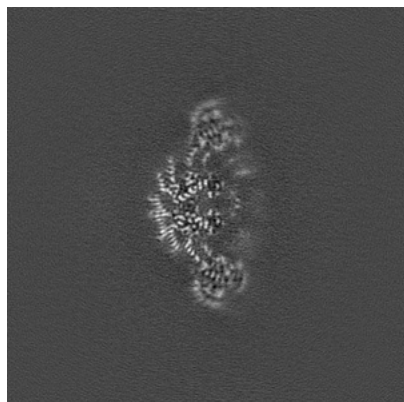


Y Index: 160

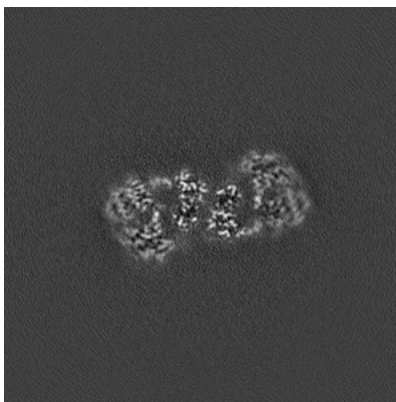


Z Index: 160

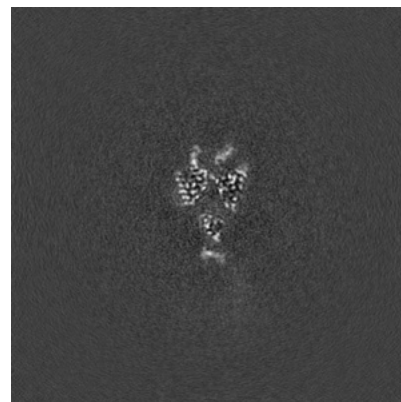
6.2.2 Raw map



X Index: 160



Y Index: 160

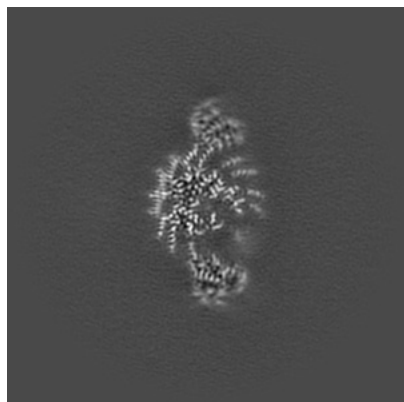


Z Index: 160

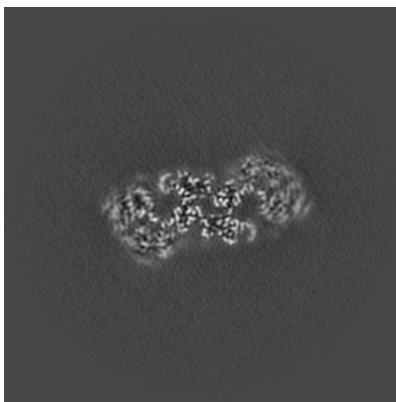
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

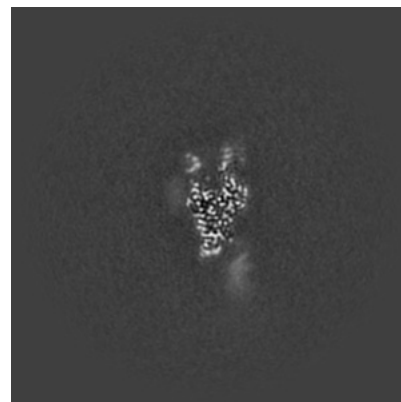
6.3.1 Primary map



X Index: 163

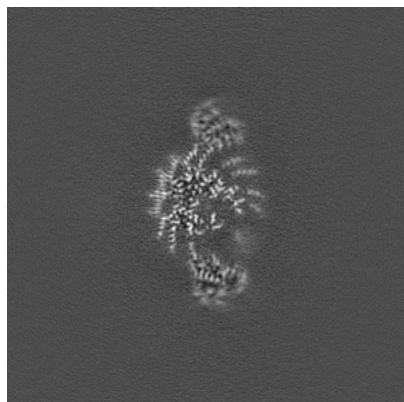


Y Index: 167

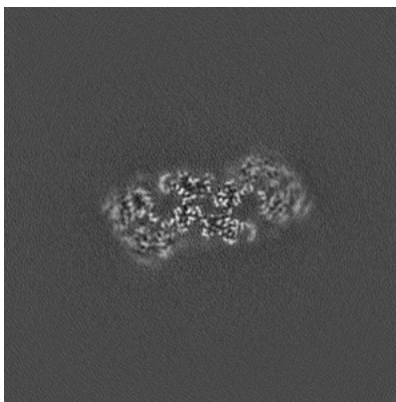


Z Index: 147

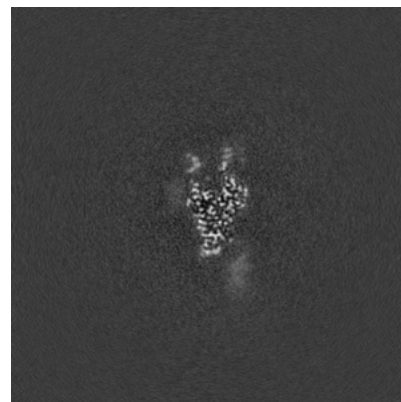
6.3.2 Raw map



X Index: 163



Y Index: 167

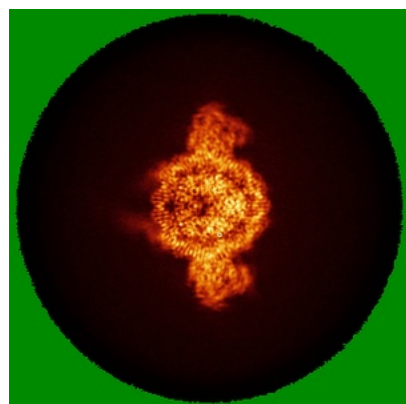


Z Index: 147

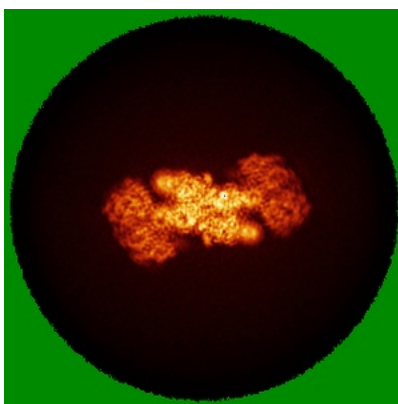
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

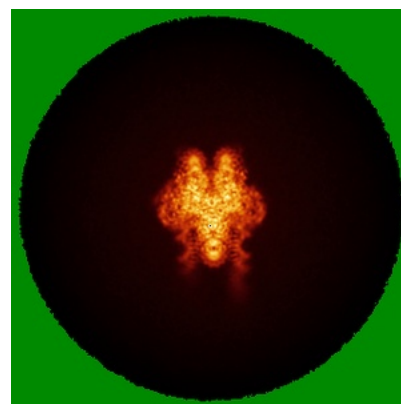
6.4.1 Primary map



X

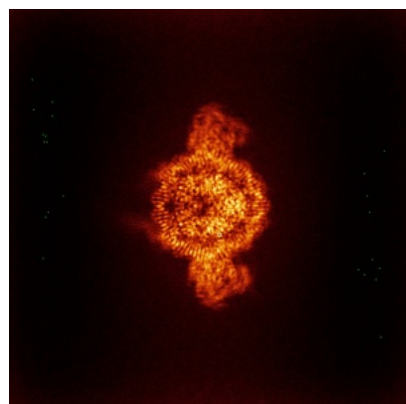


Y

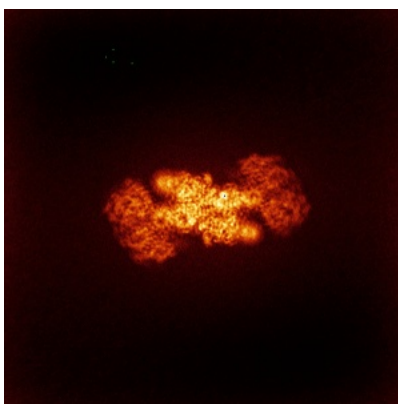


Z

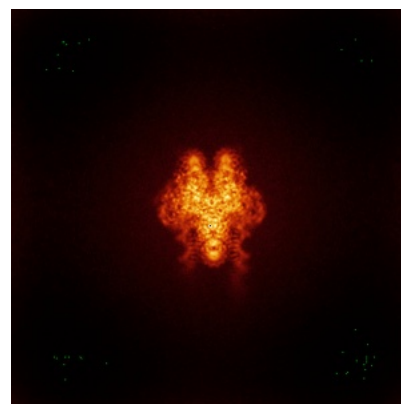
6.4.2 Raw map



X



Y

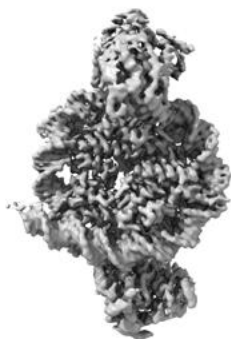


Z

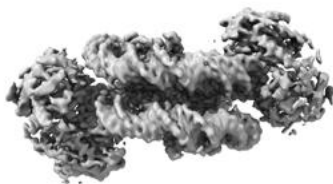
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

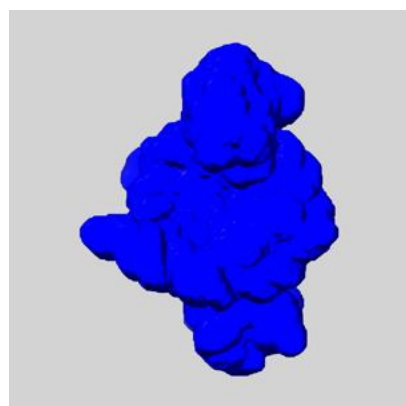
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

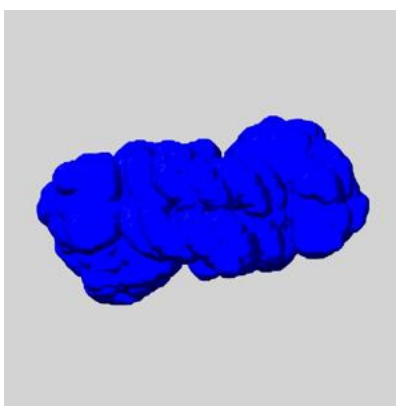
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

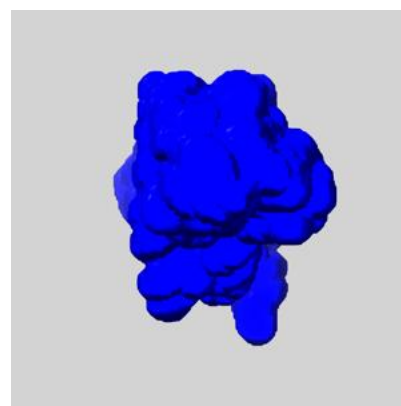
6.6.1 emd_63131_msk_1.map [i](#)



X



Y

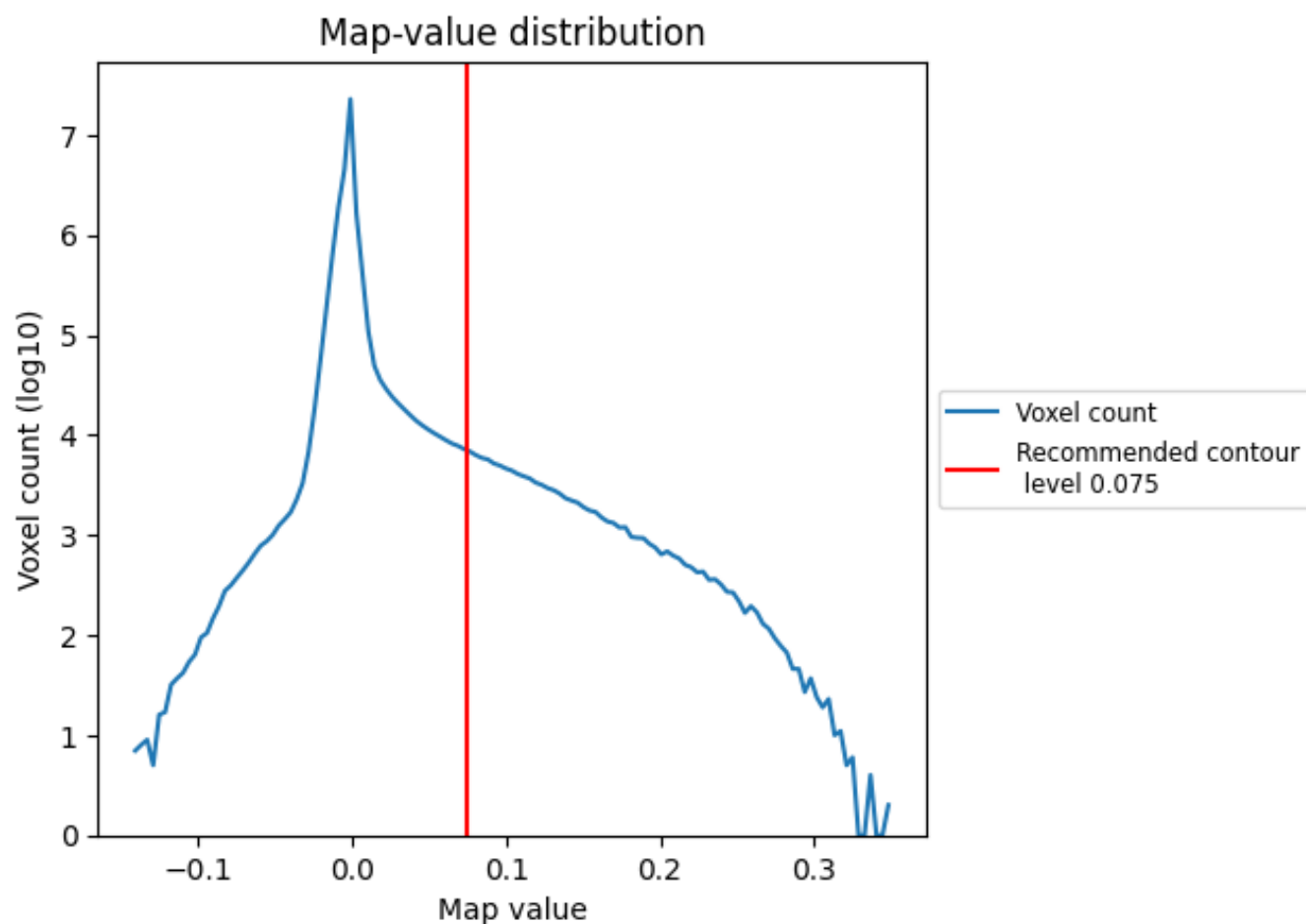


Z

7 Map analysis [i](#)

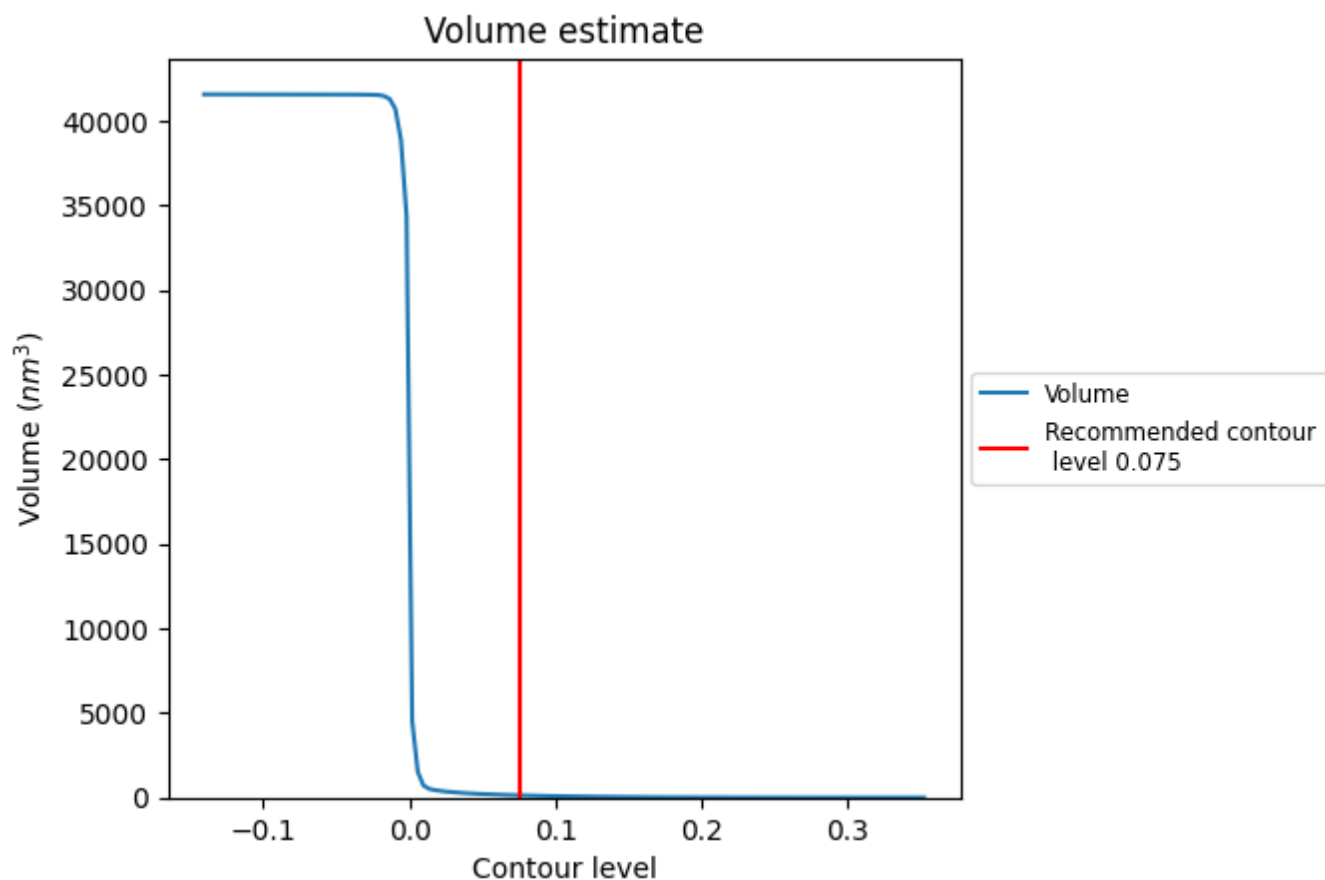
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

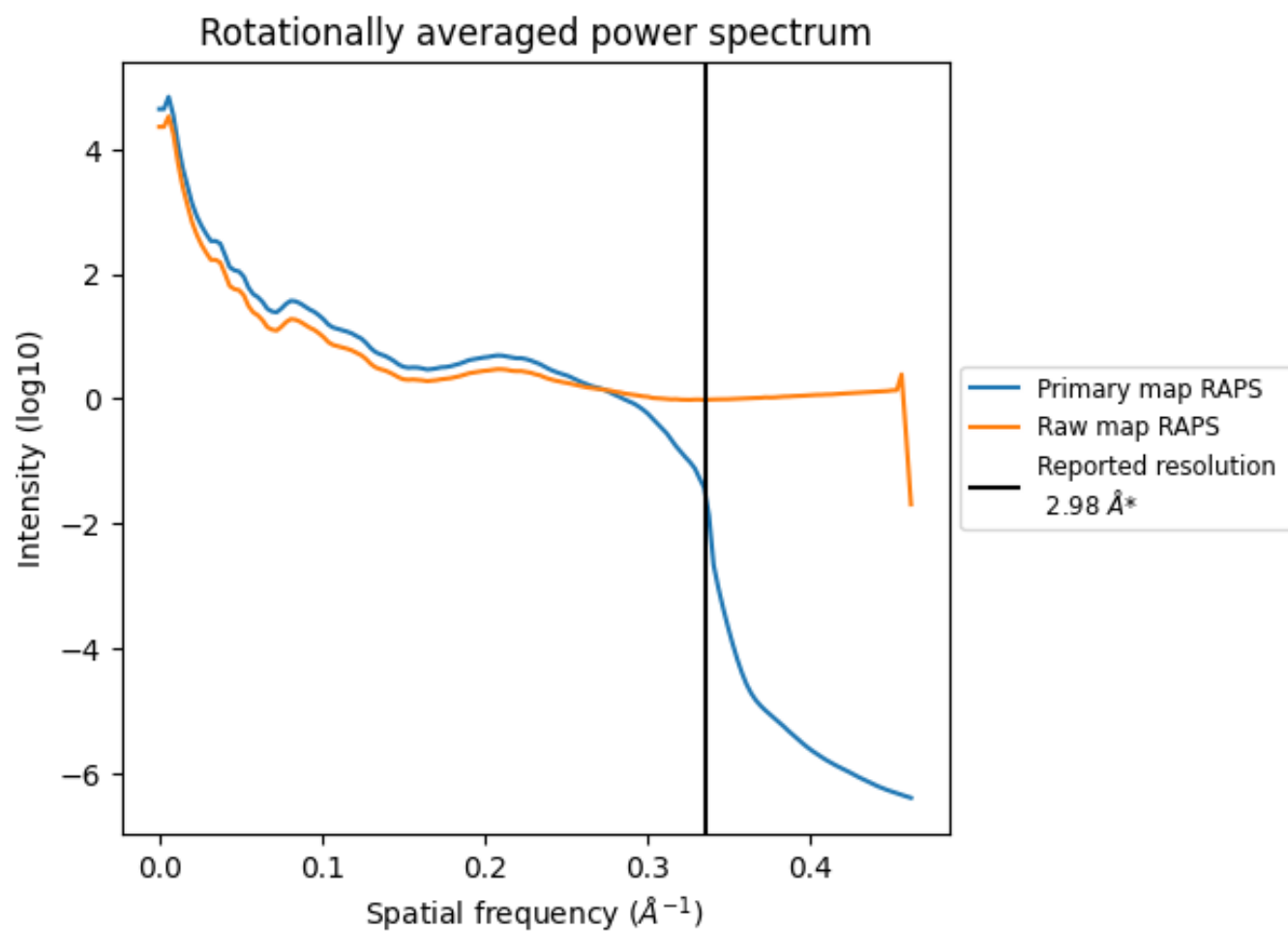
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm³; this corresponds to an approximate mass of 119 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

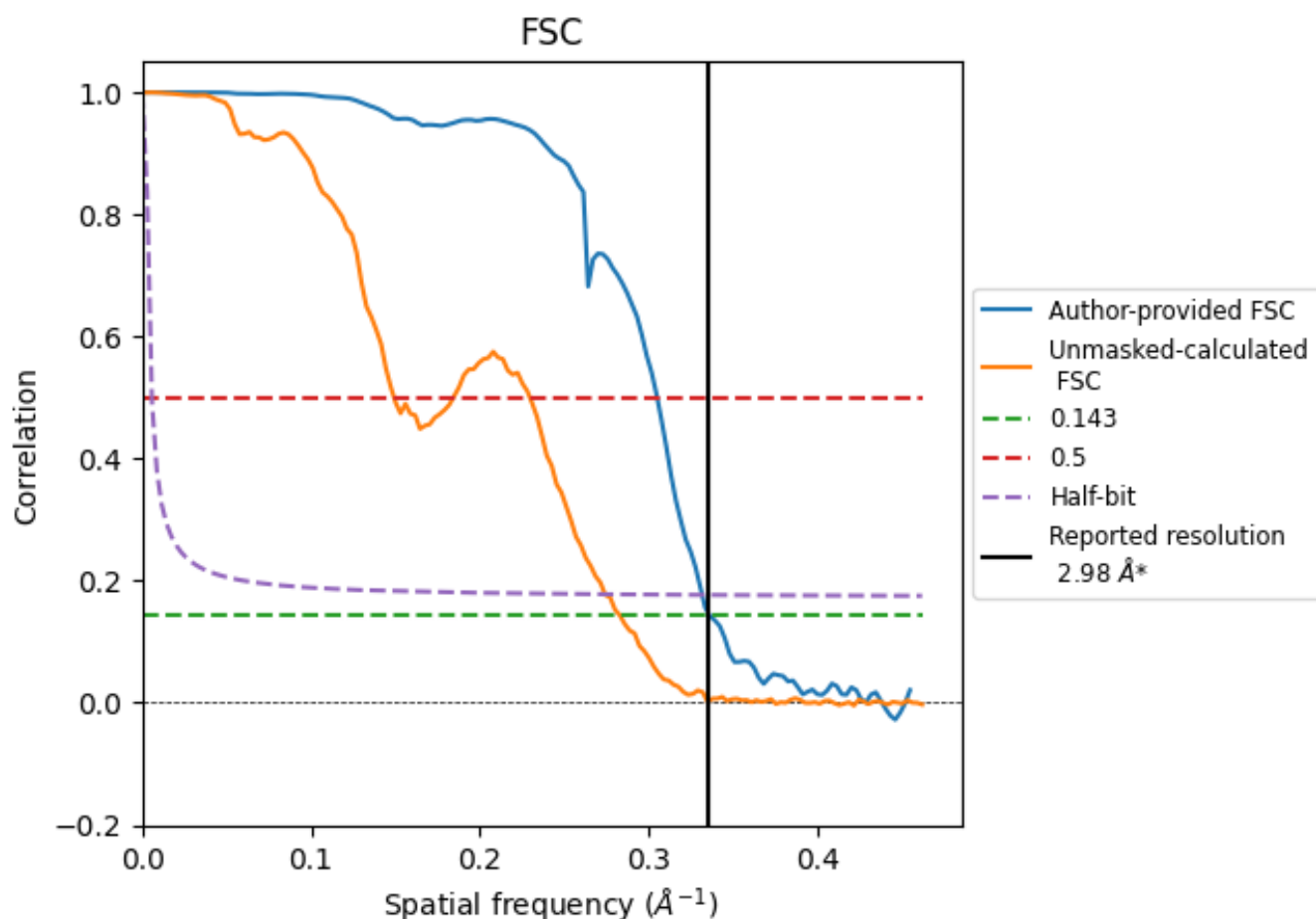


*Reported resolution corresponds to spatial frequency of $0.336 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.336 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.28	3.01
Unmasked-calculated*	3.53	6.70	3.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 2.98 by more than 10 %

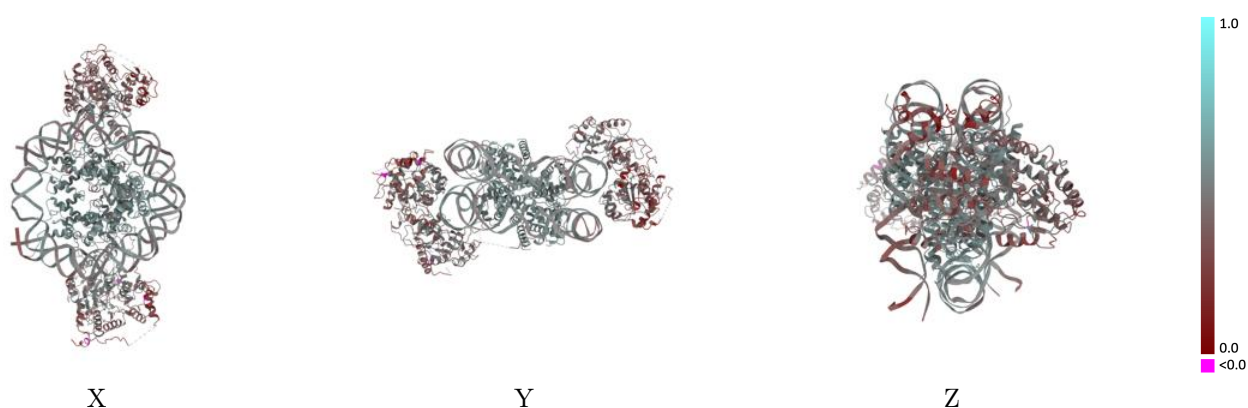
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63131 and PDB model 9LJ2. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

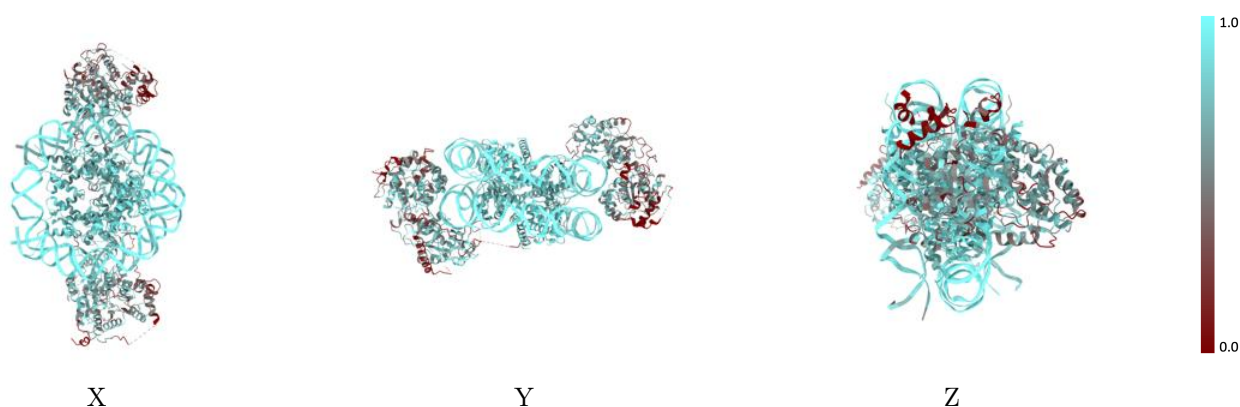
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



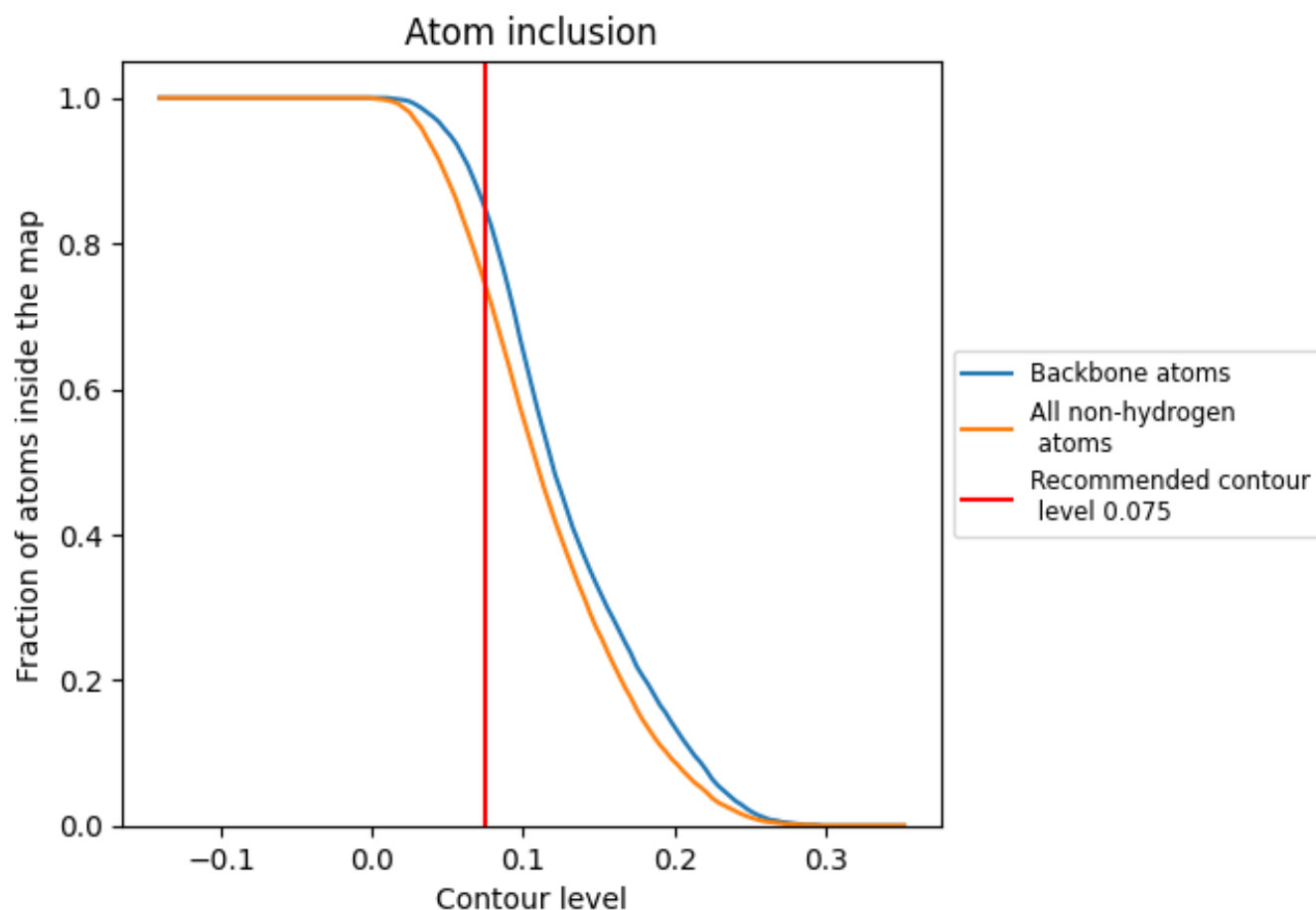
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7410	0.4580
A	0.8590	0.5470
B	0.8460	0.5450
C	0.8540	0.5490
D	0.8690	0.5440
E	0.8360	0.5360
F	0.8170	0.5330
G	0.8620	0.5520
H	0.8770	0.5390
I	0.9220	0.4860
J	0.9210	0.4810
K	0.5740	0.4020
N	0.5070	0.3630

1.0

0.0

<0.0